

Hexachloro-1,3-butadiene  
87-68-3 | DTXSID7020683

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $1.08\text{e-}12 \text{ cm}^3/\text{molecule}\cdot\text{sec}$

**Global applicability domain:** Outside

**Local applicability domain index:**  $2.64\text{e-}01$

**Confidence level:**  $6.32\text{e-}01$

## Nearest Neighbors from the Training Set

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Tetrachloroethylene

**Measured:**  $1.67\text{e-}13$

**Predicted:**  $2.29\text{e-}13$

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Trichloroethylene

**Measured:**  $2.36\text{e-}12$

**Predicted:**  $2.21\text{e-}12$

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Chloral

**Measured:**  $1.60\text{e-}12$

**Predicted:**  $1.64\text{e-}12$

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(Z)-1,2-Dichloroethylene

**Measured:**  $2.48\text{e-}12$

**Predicted:**  $2.80\text{e-}12$

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(E)-1,2-Dichloroethylene

**Measured:**  $2.48\text{e-}12$

**Predicted:**  $2.80\text{e-}12$

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Dichloroacetaldehyde

**Measured:**  $2.30\text{e-}12$

**Predicted:**  $2.47\text{e-}12$